DOES WASTE-RECYCLING REALLY IMPROVE THE MULTI-PROPOSAL METROPOLIS-HASTINGS MONTE CARLO ALGORITHM?

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Abstract. The waste-recycling Monte Carlo (WR) algorithm introduced by physicists is a modification of the (multi-proposal) Metropolis-Hastings algorithm, which makes use of all the proposals in the empirical mean, whereas the standard (multi-proposal) Metropolis-Hastings algorithm only uses the accepted proposals. In this paper, we extend the WR algorithm into a general control variate technique and exhibit the optimal choice of the control variate in terms of asymptotic variance. We also give an example which shows that in contradiction to the intuition of physicists, the WR algorithm can have an asymptotic variance larger than the one of the Metropolis-Hastings algorithm. However, in the particular case of the Metropolis-Hastings algorithm called Boltzmann algorithm, we prove that the WR algorithm is asymptotically better than the Metropolis-Hastings algorithm. This last property is also true for the multi-proposal Metropolis-Hastings algorithm. In this last framework, we consider a linear parametric generalization of WR, and we propose an estimator of the explicit optimal parameter using the proposals.

1. Introduction

The Metropolis-Hastings algorithm is used to compute the expectation $\langle \pi, f \rangle$ of a function f under a probability measure π difficult to simulate. It relies on the construction by an appropriate acceptation/rejection procedure of a Markov chain $(X_k, k \geq 0)$ with transition kernel P such that π is reversible with respect to P and the quantity of interest $\langle \pi, f \rangle$ is estimated by the empirical mean $I_n(f) = \frac{1}{n} \sum_{k=1}^{n} f(X_k)$. We shall recall the well-known properties of this estimation (consistency, asymptotic normality) in what follows. In particular the quality or precision of the algorithm is measured through the asymptotic variance of the estimator of $\langle \pi, f \rangle$.

The waste-recycling Monte Carlo (WR) algorithm, introduced by physicists, is a modification of the Metropolis-Hastings algorithm, which makes use of all the proposals in the empirical mean, whereas the standard Metropolis-Hastings algorithm only uses the accepted proposals. To our knowledge, the WR algorithm was first introduced in 1977 by Ceperley, Chester and Kalos in equation (35) p.3085 [4]. Without any proof, they claim that "The advantage of using this form is that some information about unlikely moves appears in the final answer, and the variance is lowered". It is commonly assumed among the physicists and supported by most of the simulations that the WR algorithm is more efficient than the Metropolis-Hastings algorithm, that is the estimation given by the WR algorithm is consistent and has a smaller asymptotic variance. An other way to speed up the Metropolis-Hastings algorithm could be to use multiple proposals at each step instead of only one. According to

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Frenkel [6], the waste recycling can be particularly useful for these algorithms where many states are rejected.

Our aim is to clarify the presentation of the WR algorithms with one proposal and with multiple proposals and to present a first rigorous study of those algorithms. We will give in Section 2 an introduction to our results in the finite state space case. Our main new results are stated in Theorem 3.4, which is a first step towards the comparison of the asymptotic variances. We shall detail their consequences in the didactic Section 2 for:

- the WR algorithm through Propositions 2.1 (consistency of the estimation), 2.2 (asymptotic normality) and 2.3 (a first partial answer to the initial question: Does waste-recycling really improve the Metropolis-Hastings Monte Carlo algorithm?),
- the multi-proposal WR algorithm through Propositions 2.7 (consistency of the estimation and asymptotic normality) and 2.8 (a second partial answer to the inital question: Does waste-recycling really improve the Metropolis-Hastings Monte Carlo algorithm?).

The study of the WR estimator in the form $I_n(f) + J_n(f)$, for a given functional J, leads us to rewrite the WR algorithm as a particular case of a general control variate problem by considering the estimators $I_n(f) + J_n(\psi)$ where the function ψ is possibly different from f. In the multi-proposal framework, the consistency (or convergence) of this general algorithm and its asymptotic normality are stated in Theorem 3.4 in Section 3. We also give its asymptotic variance and prove that the optimal choice of ψ in terms of asymptotic variance is the solution, F, of the Poisson equation (6). This choice achieves variance reduction, but the function F is difficult to compute. It is possible to replace it by an approximation. In some sense, f is such an approximation and for this particular choice we recover the Waste Recycling estimator introduced by physicists. In Section 5 which is dedicated to the single proposal case, we give a simple counter-example (see paragraph 5.2) which shows that the WR algorithm does not in general improve the Metropolis-Hastings algorithm : the WR algorithm can have an asymptotic variance larger than the one of the Metropolis-Hastings algorithm. Since, Athènes [3] has also observed variance augmentation in some numerical computations of free energy. However, in the particular case of the Metropolis-Hastings algorithm called Boltzmann algorithm, we prove in Section 4 that the (multi-proposal) WR algorithm is asymptotically better than the (multi-proposal) Metropolis-Hastings algorithm. In this particular framework, we explicit the optimal value $b_\star$ of b for the parametric control variate $J_n(bf)$. This optimal value can be estimated using the Makov chain $(X_k, 0 \leq k \leq n)$.

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2. Didactic version of the results

For simplicity, we assume in the present section that E is a finite set. Let $\langle \nu, h\rangle = \sum_{x\in E} \nu(x)h(x)$ denote the "integration" of a real function defined on E, $h = (h(x), x \in E)$, w.r.t. to a measure on E, $\nu = (\nu(x), x \in E)$.

Let π be a probability measure on E such that $\pi(x) > 0$ for all $x \in E$ and f a real function defined on E. The Metropolis-Hastings algorithm gives an estimation of $\langle \pi, f\rangle$ as the a.s. limit of the empirical mean of f, $\frac{1}{n}\sum_{k=1}^n f(X_k)$, as n goes to infinity, where $X = (X_n, n \geq 0)$ is a Markov chain which is reversible with respect to the probability measure π.

2.1. **The Metropolis-Hastings algorithm.** The Markov chain $X = (X_n, n \in \mathbb{N})$ of the Metropolis-Hastings algorithm is built in the following way. Let Q be an irreducible transition matrix over E such that for all $x, y \in E$, if $Q(x, y) = 0$ then $Q(y, x) = 0$. The transition matrix Q is called the selection matrix.

For $x, y \in E$ such that $Q(x, y) > 0$, let $(\rho(x, y), \rho(y, x)) \in (0, 1]^2$ be such that

$$\rho(x, y)\pi(x)Q(x, y) = \rho(y, x)\pi(y)Q(y, x). \tag{1}$$

The function ρ is viewed as an acceptance probability. For example, one gets such a function ρ by setting

$$\rho(x, y) = \gamma\left(\frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)}\right), \quad \text{for all} \quad x, y \in E \quad \text{s.t.} \quad Q(x, y) > 0, \tag{2}$$

where γ is a function with values in $(0, 1]$ such that $\gamma(u) = u\gamma(1/u)$. Usually, one takes $\gamma(u) = \min(1, u)$ for the Metropolis algorithm. The case $\gamma(u) = u/(1 + u)$ is known as the Boltzmann algorithm or Barker algorithm.

Let X_0 be a random variable taking values in E with probability distribution ν_0. At step n, $X_0, \ldots, X_n$ are given. The proposal at step $n+1$, $\tilde{X}_{n+1}$, is distributed according to $Q(X_n, \cdot)$. This proposal is accepted with probability $\rho(X_n, \tilde{X}_{n+1})$ and then $X_{n+1} = \tilde{X}_{n+1}$. If it is rejected, then we set $X_{n+1} = X_n$.

It is easy to check that $X = (X_n, n \geq 0)$ is a Markov chain with transition matrix P defined by

$$\forall x, y \in E, \quad P(x, y) = \begin{cases} Q(x, y)\rho(x, y) & \text{if } x \neq y, \\ 1 - \sum_{z \neq x} P(x, z) & \text{if } x = y. \end{cases} \tag{3}$$

Furthermore X is reversible w.r.t. to the probability measure π: $\pi(x)P(x, y) = \pi(y)P(y, x)$ for all $x, y \in E$. This property is also called detailed balance. By summation over $y \in E$, one deduces that π is an invariant probability for P (i.e. $\pi P = \pi$). The irreducibility of Q implies that P is irreducible. Since the probability measure π is invariant for P, we deduce that X is positive recurrent with (unique) invariant probability measure π. In particular, for any real valued function f defined on E, the ergodic theorem (see e.g. [8]) implies the consistency of the estimation:

$$\lim_{n\to\infty} I_n(f) = \langle \pi, f\rangle \quad \text{a.s.},$$

where

$$I_n(f) = \frac{1}{n}\sum_{k=1}^{n} f(X_k). \tag{4}$$

The asymptotic normality of the estimator $I_n(f)$ is given by the following central limit theorem (see [5] or [8])

$$\sqrt{n}\left(I_n(f) - \langle \pi, f\rangle\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0, \sigma(f)^2).$$

Here $\mathcal{N}(0, \sigma^2)$ denotes the Gaussian distribution with mean 0 and variance σ^2, the convergence holds in the distribution sense and

$$\sigma(f)^2 = \langle \pi, F^2\rangle - \langle \pi, (PF)^2\rangle. \tag{5}$$

where F denotes the unique solution up to an additive constant of the Poisson equation

$$F(x) - PF(x) = f(x) - \langle \pi, f\rangle, \quad x \in E \tag{6}$$

and $Ph(x) = \sum_{y \in E} P(x,y)h(y)$. Improving the Metropolis-Hastings algorithm means exhibiting other estimators of $\langle \pi, f\rangle$ that are still consistent (i.e. estimators which converge a.s. to $\langle \pi, f\rangle$) but with an asymptotic variance smaller than $\sigma(f)^2$.

2.2. **WR algorithm.** The classical estimation of $\langle \pi, f\rangle$ by the empirical mean $I_n(f)$ makes no use of the proposals $\tilde{X}_k$ which have been rejected. For a long time, physicists have claimed that the efficiency of the estimation can be improved by including these rejected states in the sampling procedure. They suggest to use the so-called Waste-Recycling Monte Carlo (WR) algorithm, which consists in replacing $f(X_k)$ in $I_n(f)$ by a weighted average of $f(X_{k-1})$ and $f(\tilde{X}_k)$. For the natural choice of weights corresponding to the conditional expectation of $f(X_k)$ w.r.t. $(X_{k-1}, \tilde{X}_k)$, one gets the following estimator of $\langle \pi, f\rangle$:

$$\begin{aligned} I_n^{WR}(f) &= \frac{1}{n}\sum_{k=0}^{n-1} \mathbb{E}\left[f(X_{k+1}) | X_k, \tilde{X}_{k+1}\right] \\ &= \frac{1}{n}\sum_{k=0}^{n-1} \rho(X_k, \tilde{X}_{k+1}) f(\tilde{X}_{k+1}) + (1-\rho(X_k, \tilde{X}_{k+1})) f(X_k). \end{aligned}$$

We shall study in Section 6.2 another choice for the weights also considered by Frenkel [7]. Notice that the WR algorithm requires the evaluation of f for all the proposals whereas the Metropolis-Hastings algorithm evaluates f only for the accepted proposals. Other algorithms using all the proposals, such as the Rao-Blackwell Metropolis-Hasting algorithm, have been studied, see for example section 6.4.2 in [11] and references therein. In the Rao-Blackwell Metropolis-Hasting algorithm, the weight of $f(\tilde{X}_{k+1})$ depends on all the proposals $\tilde{X}_1, \ldots, \tilde{X}_n$. It is thus necessary to keep in memory the values of all proposals in order to compute the estimation of $\langle \pi, f\rangle$.

One easily checks that $I_n^{WR}(f) - I_n(f) = J_n(f)$ where for any real function ψ defined on E,

$$\begin{aligned} J_n(\psi) &= \frac{1}{n}\sum_{k=0}^{n-1} \left(\mathbb{E}\left[\psi(X_{k+1}) | X_k, \tilde{X}_{k+1}\right] - \psi(X_{k+1}) \right) \\ &= \frac{1}{n}\sum_{k=0}^{n-1} \left(\rho(X_k, \tilde{X}_{k+1}) \psi(\tilde{X}_{k+1}) + (1-\rho(X_k, \tilde{X}_{k+1})) \psi(X_k) - \psi(X_{k+1}) \right). \end{aligned}$$

Notice that $J_n(\psi) = 0$ when ψ is constant. We can consider a more general estimator of $\langle \pi, f\rangle$ given by

$$I_n(f, \psi) = I_n(f) + J_n(\psi).$$

Notice that $I_n^{WR}(f) = I_n(f,f)$ and $I_n(f) = I_n(f,0)$. It is easy to check that the bias of the estimator $I_n(f,\psi)$ does not depend on ψ: $\mathbb{E}[I_n(f,\psi)] = \mathbb{E}[I_n(f)]$. Theorem 3.4 implies the following result on the estimator $I_n(f,\psi)$.

Proposition 2.1. *For any real functions ψ and f defined on E, the estimator $I_n(f,\psi)$ of $\langle \pi, f\rangle$ is consistent: a.s.* $\lim_{n\to\infty} I_n(f,\psi) = \langle \pi, f\rangle$.

From this result, $J_n(\psi)$ can be seen as a control variate and it is natural to look for ψ which minimizes the variance or the asymptotic variance of $I_n(f,\psi)$. Another class of control variates has been studied in [2] in the particular case of the Independent Metropolis-Hastings algorithm where $Q(x,.)$ does not depend on x.

The last part of Theorem 3.4 implies the following result, where we used Lemma 5.1 to derive the asymptotic variance expression. We shall write $\mathbb{E}_\pi$ when X_0 is distributed under its invariant measure π (in particular $\langle \pi, f\rangle = \mathbb{E}_\pi[f(X_0)]$).

Proposition 2.2. *For any real functions ψ and f defined on E, the estimator $I_n(f,\psi)$ of $\langle \pi, f\rangle$ is asymptotically normal:*

$$\sqrt{n}\,(I_n(f,\psi) - \langle \pi, f\rangle) \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0, \sigma(f,\psi)^2),$$

with asymptotic variance $\sigma(f,\psi)^2$ given by

$$\sigma(f,\psi) = \sigma(f)^2 - \mathbb{E}_\pi\left[\Big(1-\rho(X_0,X_1)\Big)\Big(F(X_1)-F(X_0)\Big)^2\right] + \mathbb{E}_\pi\left[\Big(1-\rho(X_0,X_1)\Big)\Big(\psi(X_1)-F(X_1)-\psi(X_0)+F(X_0)\Big)^2\right],$$

where F solves the Poisson equation (6). In particular, for fixed f, the asymptotic variance $\sigma(f,\psi)^2$ is minimal for $\psi = F$ and this choice achieves variance reduction : $\sigma(f,F)^2 \le \sigma(f)^2$.

Although optimal in terms of the asymptotic variance, the estimator $I_n(f,F)$ is not for use in practice, since computing a solution of the Poisson equation is more complicated than computing $\langle \pi, f\rangle$. Nevertheless, the Proposition suggests that using $I_n(f,\psi)$ where ψ is an approximation of F might lead to a smaller asymptotic variance than in the standard Metropolis-Hastings algorithm. Some hint at the computation of an approximation of F by a Monte Carlo approach is for instance given in [9] p.418-419. Because of the series expansion $F = \sum_{k\ge 0} P^k(f - \langle \pi, f\rangle)$, f can be seen as an approximation of F of order 0. Hence the asymptotic variance of $I_n^{WR}(f) = I_n(f,f)$ might be smaller than the one of $I_n(f)$ in some situations. It is common belief in the physicist community, see [4] or [7], that the inequality is always true. Notice that, as remarked by Frenkel in a particular case [7], the variance of each term of the sum in $I_n^{WR}(f)$ is equal or smaller than the variance of each term of the sum in $I_n(f)$ by Jensen inequality. But one has also to compare the covariance terms, which is not so obvious. We investigate whether the asymptotic variance of the WR algorithm is smaller than the one of the standard Metropolis algorithm and reach the following conclusion which contradicts the intuition.

Proposition 2.3.

i) *In the Metropolis case, that is when* (2) *holds with $\gamma(u) = \min(1,u)$, then it may happen that $\sigma(f,f)^2 > \sigma(f)^2$.*

ii) *When* (2) *holds with $\gamma(u) = \dfrac{\alpha u}{1+u}$, for some $\alpha \in (0,2)$, then we have $\sigma(f,f)^2 \le \sigma(f)^2$. Furthermore, for f non constant, the function $b \mapsto \sigma(f,bf)^2$ is minimal at*

$$b_\star = \frac{\langle \pi, f^2\rangle - \langle \pi, f\rangle^2}{\langle \pi, f^2 - fPf\rangle} \tag{7}$$

and $b_\star \ge 1/\alpha$. When $\alpha = 1$, if, moreover, $\sigma(f,f)^2 > 0$, then $b_\star > 1$.

Remark 2.4. Assume that f is not constant. The optimal parameter $b_\star$ defined by (7) can be estimated by

$$\hat{b}_n = \frac{I_n(f^2) - I_n(f)^2}{I_n(f^2) - \frac{1}{n}\sum_{k=1}^n f(X_{k-1})f(X_k)}.$$

Notice that a.s. $\lim_{n\to\infty} \hat{b}_n = b_\star$ thanks to the ergodic theorem. Using Slutsky theorem, one can deduce from Proposition 2.2 that $I_n(f) + \hat{b}_n J_n(f) = I_n(f, \hat{b}_n f)$ is an asymptotically normal estimator of $\langle \pi, f\rangle$ with asymptotic variance $\sigma(f, b_\star f)^2$. Thus, in the framework ii) of Proposition 2.3, using the control variate $\hat{b}_n J_n(f)$ improves strictly the WR estimator as soon as either $\alpha < 1$ or $\alpha = 1$ (Boltzmann algorithm) and $\sigma(f, f)^2$ is positive. Notice that when its asymptotic variance $\sigma(f, f)^2$ is zero, then the WR estimator $I_n^{WR}(f) = I_n(f, f)$ is equal to $\langle \pi, f\rangle$. $\lozenge$

To prove assertion i), we give an explicit counter-example such that $\sigma(f, f)^2 > \sigma(f)^2$ in the Metropolis case (see Section 5.2 and equation (32)). The assertion ii) is also proved in Section 5 (see Proposition 5.3). Let us make some comments on its hypothesis which holds with $\alpha = 1$ for Boltzmann acceptation rule.

- By (1) and since $\rho(x, y)$ is an acceptance probability, the constant α has to be smaller than $1 + \min_{x\neq y, Q(x,y)>0} \dfrac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)}$.
- If there exists a constant $c > 0$ s.t. for all distinct $x, y \in E$ s.t. $Q(x, y) > 0$, the quantity $\dfrac{\pi(x)Q(x, y)}{\pi(y)Q(y, x)}$ is equal to c or $1/c$ and (2) holds with γ such that $\gamma(1/c) = \gamma(c)/c$ then the hypothesis holds with $\alpha = \gamma(c) + \gamma(1/c)$. For example assume that the transition matrix Q is symmetric and that π is written as a Gibbs distribution: for all $x \in E$, $\pi(x) = \mathrm{e}^{-H(x)} / \sum_{y\in E} \mathrm{e}^{-H(y)}$ for some energy function H. If the energy increases or decreases by the same amount ε for all the authorized transitions, then $\dfrac{\pi(x)Q(x, y)}{\pi(y)Q(y, x)}$ is equal to c or $1/c$ with $c = e^\varepsilon$.

According to [10], since for all $u > 0$, $\dfrac{u}{1+u} < \min(1, u)$, in the absence of waste recycling, the asymptotic variance $\sigma(f)^2$ is smaller in the Metropolis case than in the Boltzmann case for given π, Q and f. So waste recycling always achieves variance reduction only for the worst choice of γ. Notice however that the Boltzmann algorithm is used in the multi-proposal framework where we generalize our results.

Remark 2.5. When the computation of Pg is feasible for any function $g : E \to \mathbb{R}$ (typically when, for every $x \in E$, the cardinal of $\{y \in E : Q(x, y) > 0\}$ is small), then it is possible to use $I_n(\psi - P\psi)$ as a control variate and approximate $\langle \pi, f\rangle$ by $I_n(f - (\psi - P\psi))$. Since π is invariant with respect to P, $\langle \pi, \psi - P\psi\rangle = 0$ and a.s. $I_n(f - (\psi - P\psi))$ converges to $\langle \pi, f\rangle$ as n tends to infinity. Moreover, the asymptotic variance of the estimator is $\sigma(f - \psi + P\psi)^2$. Last, remarking that

$$I_n(\psi - P\psi) = \frac{1}{n}\sum_{k=1}^{n} (\psi(X_k) - P\psi(X_{k-1})) + \frac{1}{n} (P\psi(X_0) - P\psi(X_n)) \tag{8}$$

one obtains that the bias difference $\mathbb{E}[I_n(f - \psi + P\psi)] - \mathbb{E}[I_n(f)] = \frac{1}{n}\mathbb{E}\left[P\psi(X_0) - P\psi(X_n)\right]$ is smaller than $2\max_{x\in E} |\psi(x)|/n$.

For the choice $\psi = F$, this control variate is perfect, since according to (6), for each $n \in \mathbb{N}^*$, $I_n(f - (F - PF))$ is constant and equal to $\langle \pi, f\rangle$.

For the choice $\psi = f$, the asymptotic variance of the estimator $I_n(Pf)$ is also smaller than the one of $I_n(f)$. Indeed setting $f_0 = f - \langle \pi, f \rangle$, we have

$$\begin{aligned}\sigma(f)^2 - \sigma(Pf)^2 &= \langle \pi, F^2 + (P^2F)^2 - 2(PF)^2 \rangle \\ &= \langle \pi, (f_0 + PF)^2 - 2(PF)^2 + (Pf_0 - PF)^2 \rangle \\ &= \langle \pi, f_0^2 + 2f_0P(F - PF) + (Pf_0)^2 \rangle = \langle \pi, (f_0 + Pf_0)^2 \rangle\end{aligned}$$

where we used that PF solves the Poisson equation (6) with f replaced by Pf and (5) for the first equality, (6) for the second and last equalities and the reversibility of π w.r.t. P for the last one.

Notice the control variate $J_n(\psi)$ is similar to $I_n(\psi - P\psi)$ except that the conditional expectation $P\psi(X_{k-1})$ of $\psi(X_k)$ given X_{k-1} in the first term of the r.h.s. of (8) is replaced by the conditional expectation of $\psi(X_k)$ given $(X_{k-1}, \tilde{X}_k)$ which can always be easily computed. From this perspective, the minimality of the asymptotic variance of $I_n(f, \psi)$ for $\psi = F$ is not a surprise.

The comparison between $\sigma(f, \psi)^2$ and $\sigma(f - \psi + P\psi)^2$ can be deduced from Section 6.1 which is stated in the more general multi-proposal framework introduced in the next paragraph. Notice that the sign of $\sigma(f, \psi)^2 - \sigma(f - \psi + P\psi)^2$ depends on ψ. $\lozenge$

2.3. **Multi-proposal WR algorithm.** In the classical Metropolis Hasting algorithm, there is only one proposal $\tilde{X}_{n+1}$ at step $n + 1$. Around 1990, some extensions where only one state among multiple proposals is accepted have been proposed in order to speed up the exploration of E (see [1] for a unifying presentation of MCMC algorithms including the multi-proposal Metropolis Hasting algorithm). According to Frenkel [6], the waste recycling can be particularly useful for these algorithms where many states are rejected.

To formalize these algorithms, we introduce a proposition kernel $\mathcal{Q} : E \times \mathcal{P}(E) \to [0, 1]$, where $\mathcal{P}(E)$ denotes the set of parts of E, which describes how to randomly choose the set of proposals:

$$\forall x \in E,\ \mathcal{Q}(x, A) = 0 \text{ if } x \notin A \quad \text{and} \quad \sum_{A \in \mathcal{P}(E)} \mathcal{Q}(x, A) = 1. \tag{9}$$

The second condition says that $\mathcal{Q}(x, \cdot)$ is a probability on $\mathcal{P}(E)$. The first one ensures that the starting point is among the proposals. This last convention will allow us to transform the rejection/acceptation procedure into a selection procedure among the proposals.

The selection procedure is described by a probability κ. For $(x, A) \in E \times \mathcal{P}(E)$, let $\kappa(x, A, \tilde{x}) \in [0, 1]$ denote the probability of choosing $\tilde{x} \in A$ as the next state when the proposal set A has been chosen. We assume that $\sum_{\tilde{x} \in A} \kappa(x, A, \tilde{x}) = 1$ (that is $\kappa(x, A, \cdot)$ is a probability measure) and that the following condition holds :

$$\forall A \in \mathcal{P}(E),\ \forall x, \tilde{x} \in A,\ \pi(x)\mathcal{Q}(x, A)\kappa(x, A, \tilde{x}) = \pi(\tilde{x})\mathcal{Q}(\tilde{x}, A)\kappa(\tilde{x}, A, x). \tag{10}$$

This condition is the analogue of (1) for a multi-proposal setting. For examples of non-trivial selection probability κ, see after Proposition 2.7.

The Markov chain $X = (X_n, n \geq 0)$ is now defined inductively in the following way. Let X_0 be a random variable taking values in E with probability distribution ν_0. At step n, $X_0, \ldots, X_n$ are given. The proposal set at step $n + 1$, A_{n+1}, is distributed according to $\mathcal{Q}(X_n, \cdot)$. Then X_{n+1} is chosen distributed according to $\kappa(X_n, A_{n+1}, .)$. It is easy to check that X is a Markov chain with transition matrix

$$P(x, y) = \sum_{A \in \mathcal{P}(E): x, y \in A} \mathcal{Q}(x, A)\kappa(x, A, y). \tag{11}$$

Condition (10) ensures that X is reversible w.r.t. the probability measure π : $\pi(x)P(x,y) = \pi(y)P(y,x)$.

Remark 2.6. The multi-proposal Metropolis-Hastings algorithm generalizes the Metropolis-Hastings algorithm which can be recovered for the particular choice $\mathcal{Q}(x,\{x,y\}) = Q(x,y)$ and for $y \neq x$, $\kappa(x,\{x,y\},y) = 1 - \kappa(x,\{x,y\},x) = \rho(x,y)$. ◊

We keep the definition (4) of $I_n(f)$ but adapt the ones of $J_n(\psi)$ and $I_n(f,\psi)$ as follows :

$$\begin{aligned}\mathcal{J}_n(\psi) &= \frac{1}{n}\sum_{k=0}^{n-1}\Big(\mathbb{E}\left[\psi(X_{k+1})|X_k, A_{k+1}\right] - \psi(X_{k+1})\Big)\\ &= \frac{1}{n}\sum_{k=0}^{n-1}\Big(\sum_{\tilde{x}\in A_{k+1}}\kappa(X_k, A_{k+1}, \tilde{x})\psi(\tilde{x}) - \psi(X_{k+1})\Big)\end{aligned} \tag{12}$$

and $\mathcal{I}_n(f,\psi) = I_n(f) + \mathcal{J}_n(\psi)$. The Waste Recycling estimator of $\langle\pi, f\rangle$ studied by Frenkel in [6] is given by $\mathcal{I}_n^{WR}(f) = \mathcal{I}_n(f,f)$. Notice that the bias of the estimator $\mathcal{I}_n(f,\psi)$ does not depend on ψ (i.e. $\mathbb{E}[\mathcal{I}_n(f,\psi)] = \mathbb{E}[I_n(f)]$). It turns out that Propositions 2.1 and 2.2 remain true in this multi-proposal framework (see Theorem 3.4) as soon as P is irreducible. Notice that the irreducibility of P holds if and only if for all $x' \neq y \in E$, there exist $m \geq 1$, distinct $x_0 = y, x_1, x_2, \ldots, x_m = x' \in E$ and $A_1, A_k \ldots, A_m \in \mathcal{P}(E)$ such that for all $k \in \{1,\ldots,m\}$, $x_{k-1}, x_k \in A_k$ and

$$\prod_{k=1}^{m}\mathcal{Q}(x_{k-1}, A_k)\kappa(x_{k-1}, A_k, x_k) > 0. \tag{13}$$

Proposition 2.7. *Assume that P is irreducible. For any real functions ψ and f defined on E, we have:*

- *The estimator $\mathcal{I}_n(f,\psi)$ of $\langle\pi, f\rangle$ is consistent: a.s. $\lim_{n\to\infty}\mathcal{I}_n(f,\psi) = \langle\pi, f\rangle$.*
- *The estimator $\mathcal{I}_n(f,\psi)$ of $\langle\pi, f\rangle$ is asymptotically normal:*
$$\sqrt{n}\left(\mathcal{I}_n(f,\psi) - \langle\pi, f\rangle\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0, \sigma(f,\psi)^2)$$
where the asymptotic variance (still denoted by) $\sigma(f,\psi)^2$ is given by
$$\sigma(f,\psi)^2 = \sigma(f)^2 + \sum_{x\in E, A\in\mathcal{P}(E)}\pi(x)\mathcal{Q}(x,A)\left[\mathrm{Var}_{\kappa_{x,A}}(\psi - F) - \mathrm{Var}_{\kappa_{x,A}}(F)\right],$$
with $\mathrm{Var}_{\kappa_{x,A}}(g) = \sum_{y\in A}\kappa(x,A,y)g(y)^2 - \left(\sum_{y\in A}\kappa(x,A,y)g(y)\right)^2$.
- *Moreover, for fixed f, the asymptotic variance $\sigma(f,\psi)^2$ is minimal for $\psi = F$ where F solves the Poisson equation (6). In particular, this choice achieves variance reduction: $\sigma(f,F)^2 \leq \sigma(f)^2$.*

We now give two examples of non-trivial selection probability κ which satisfies condition (10). The first one, κ^M, defined by

$$\kappa^M(x,A,\tilde{x}) = \begin{cases}\dfrac{\pi(\tilde{x})\mathcal{Q}(\tilde{x},A)}{\max\left(\pi(\tilde{x})\mathcal{Q}(\tilde{x},A), \pi(x)\mathcal{Q}(x,A)\right) + \sum_{z\in A\setminus\{x,\tilde{x}\}}\pi(z)\mathcal{Q}(z,A)} & \text{if } \tilde{x}\neq x,\\ 1 - \sum_{z\in A\setminus\{x\}}\kappa^M(x,A,z) & \text{if } \tilde{x} = x,\end{cases} \tag{14}$$

generalizes the Metropolis selection given by (2) with $\gamma(u) = \min(1, u)$. (Notice that for $x \neq \tilde{x}$ one has $\kappa^M(x, A, \tilde{x}) \leq \dfrac{\pi(\tilde{x})\mathcal{Q}(\tilde{x}, A)}{\sum_{z\in A\setminus\{x\}} \pi(z)\mathcal{Q}(z, A)}$, which implies that $1 - \sum_{z\in A\setminus\{x\}} \kappa^M(x, A, z)$ is indeed non-negative.) The second one, κ^B, which does not depend on the initial point x, and is defined by

$$\kappa^B(x, A, \tilde{x}) = \kappa^B(A, \tilde{x}) = \frac{\pi(\tilde{x})\mathcal{Q}(\tilde{x}, A)}{\sum_{z\in A} \pi(z)\mathcal{Q}(z, A)}, \tag{15}$$

generalizes the Boltzmann (or Barker) selection given by (2) with $\gamma(u) = \dfrac{u}{1+u}$. Notice that for both choices, the irreducibility condition (13) can be expressed only in terms of $\mathcal{Q}$:

$$\prod_{k=1}^{m} \mathcal{Q}(x_{k-1}, A_k)\mathcal{Q}(x_k, A_k) > 0.$$

For the selection probability (15), we prove in section 4 (see Proposition 4.1) that the Waste Recycling improves the Metropolis-Hasting algorithm :

Proposition 2.8. *When $\kappa = \kappa^B$ is given by* (15) *(Boltzmann or Barker case), then we have $\sigma(f, f)^2 \leq \sigma(f)^2$. Furthermore, for f non constant, the function $b \mapsto \sigma(f, bf)^2$ is minimal at $b_\star$ defined by (7) and $b_\star > 1$ when $\sigma(f, f)^2 > 0$.*

Since for $\tilde{x} \neq x \in A$, $\kappa^M(x, A, \tilde{x}) \geq \kappa^B(A, \tilde{x})$, according to [10], the asymptotic variance $\sigma(f)^2$ remains smaller in the Metropolis case than in the Boltzmann one. Nethertheless, it is likely that the difference decreases when the cardinality of the proposal sets increases. Notice that the optimal value $b_\star$ can be estimated by $\hat{b}_n$ which is computed using the proposals: see Remark 2.4. The control variate $\hat{b}_n J_n(f)$ improves therefore the WR algorithm.

3. Main result for general multi-proposal WR

Let $(E, \mathcal{F}_E)$ be a measurable space s.t. $\{x\} \in \mathcal{F}_E$ for all $x \in E$, and π be a probability measure on E. Notice that E is not assumed to be finite. Let $\mathcal{P} = \{A \subset E; \text{Card}\,(A) < \infty\}$ be the set of finite subsets of E. Let $\bar{E} = \cup_{n\geq 1} E^n$ and $\mathcal{F}_{\bar{E}}$ the smallest σ-field on $\bar{E}$ which contains $A_1 \times \cdots \times A_n$ for all $A_i \in \mathcal{F}_E$ and $n \geq 1$. We consider the function Γ defined on $\bar{E}$ taking value on $\mathcal{P}$ such that $\Gamma((x_1, \ldots, x_n))$ is the set $\{x_1, \ldots, x_n\}$ of distinct elements in $(x_1, \ldots, x_n)$. We define $\mathcal{F}_{\mathcal{P}}$, a σ-field on $\mathcal{P}$, as the image of $\mathcal{F}_{\bar{E}}$ by the application Γ. We consider a measurable proposition probability kernel $\mathcal{Q} : E \times \mathcal{F}_{\mathcal{P}} \to [0, 1]$ s.t.

$$\int_{\mathcal{P}} \mathcal{Q}(x, dA) = 1 \quad \text{and} \quad \int_{\mathcal{P}} \mathcal{Q}(x, dA)\, \mathbf{1}_{\{x \notin A\}} = 0 \tag{16}$$

(this is the analogue of (9)) and a measurable selection probability kernel $\kappa : E \times \mathcal{P} \times \mathcal{F}_E \to [0, 1]$ s.t. for $x \in A$ we have $\kappa(x, A, A) = 1$. Let δ_y be the Dirac mass at point y. In particular, since A is finite, with a slight abuse of notation, we shall also write $\kappa(x, A, dy) = \sum_{z\in A} \kappa(x, A, z)\delta_z(dy)$ and so $\sum_{y\in A} \kappa(x, A, y) = 1$.

We assume that the analogue of (10) holds, that is

$$\pi(dx)\mathcal{Q}(x, dA)\kappa(x, A, dy) = \pi(dy)\mathcal{Q}(y, dA)\kappa(y, A, dx). \tag{17}$$

Example 3.1. We give the analogue of the Metropolis and Boltzmann selection kernel defined in (14) and (15) when E is finite. We consider $N(dx, dA) = \pi(dx)\mathcal{Q}(x, dA)$ and a measure $N_0(dA)$ on $\mathcal{F}_{\mathcal{P}}$ such that $\int_{x\in E} N(dx, dA)$ is absolutely continuous w.r.t. $N_0(dA)$. Since $x \in A$ and A is finite $N(dx, dA)$-a.s., the decomposition of N w.r.t. N_0 gives that $N(dx, dA) =$

$N_0(dA)r_A(dx)$, where $r_A(dx) = \sum_{y\in A} r_A(y)\delta_y(dx)$ if A is finite and $r_A(dx) = 0$ otherwise, and $(x, A) \mapsto r_A(x)$ is jointly measurable.

The Metropolis selection kernel is given by: for $x, y \in A$, $r_A \neq 0$,

$$\kappa^M(x, A, y) = \frac{r_A(y)}{\sum_{z\in A\setminus\{x,y\}} r_A(z) + \max(r_A(x), r_A(y))}, \tag{18}$$

if $x \neq y$ and $\kappa^M(x, A, x) = 1 - \sum_{y\in A\setminus\{x\}} \kappa^M(x, A, y)$.

The Boltzmann selection kernel is given by: for $x, y \in A$, $r_A \neq 0$,

$$\kappa^B(x, A, y) = \kappa^B(A, y) = \frac{r_A(y)}{\sum_{z\in A} r_A(z)}. \tag{19}$$

We choose those two selection kernels to be equal to the uniform distribution on A when $r_A = 0$. For those two selection kernels, equation (17) is satisfied. △

Example 3.2. Let us give a natural example. Let ν be a reference measure on E with no atoms, π a probability measure on E with density w.r.t. ν which we still denote by π, a selection procedure given by $\mathcal{Q}(x, \mathcal{A}) = \mathbb{P}_x(\{x, Y_1, \dots, Y_n\} \subset \mathcal{A})$ for $\mathcal{A} \in \mathcal{F}_\mathcal{P}$, where $Y_1, \dots, Y_n$ are E-valued independent random variables with density w.r.t. ν given by $q(x, \cdot)$ under $\mathbb{P}_x$ and $n \geq 1$ is fixed. We use notations of Example 3.1. In this setting, we choose $N_0(dA) = \prod_{x\in A} \nu(dx)$ and the function r_A is given by: for $x \in A$, $r_A(x) = \pi(x) \displaystyle\prod_{z\in A\setminus\{x\}} q(x, z)$. △

The Markov chain $X = (X_n, n \geq 0)$ is defined inductively in the following way. Let X_0 be a random variable taking values in E with probability distribution ν_0. At step n, $X_0, \dots, X_n$ are given. The proposal set at step $n + 1$, A_{n+1}, is distributed according to $\mathcal{Q}(X_n, \cdot)$. Then X_{n+1} is chosen distributed according to $\kappa(X_n, A_{n+1}, .)$. This is a particular case of the hit and run algorithm [1], where the proposal sets are always finite. It is easy to check that X is a Markov chain with transition kernel

$$P(x, dy) = \int_\mathcal{P} \mathcal{Q}(x, dA)\kappa(x, A, dy). \tag{20}$$

For f a real valued measurable function defined on E, we shall write $Pf(x)$ for $\int_E P(x, dy)f(y)$ when this integral is well defined.

Condition (17) ensures that X is reversible w.r.t. π : $\pi(dx)P(x, dy) = \pi(dy)P(y, dx)$. We also assume that X is Harris recurrent (see [8] section 9). This is equivalent to assume that for all $B \in \mathcal{F}_E$ s.t. $\pi(B) > 0$ we have $\mathbb{P}(\text{Card } \{n \geq 0; X_n \in B\} = \infty | X_0 = x) = 1$ for all $x \in E$.

Example 3.3. It is easy to check in Example 3.2 that X is Harris recurrent if the random walk with transition kernel q is itself Harris recurrent and

$$\forall x \in E,\ \mathcal{Q}(x, dA) \text{ a.e. },\ \forall y \in A,\ \kappa(x, A, y) > 0.$$

△

For f a real valued measurable function defined on E and ν a measure on E, we shall write $\langle \nu, f\rangle$ for $\int \nu(dy)f(y)$ when this integral is well defined.

Let f be a real-valued measurable function defined on E s.t. $\langle \pi, |f|\rangle < \infty$. Theorem 17.3.2 in [8] asserts that a.s. $\lim_{n\to\infty} I_n(f) = \langle \pi, f\rangle$, with $I_n(f)$ defined by (4).

We consider the functional $\mathcal{J}_n$ defined by

$$\mathcal{J}_n(\beta) = \frac{1}{n}\sum_{k=0}^{n-1}\Big(\mathbb{E}\left[\beta(X_k, A_{k+1}, X_{k+1})|X_k, A_{k+1}\right] - \beta(X_k, A_{k+1}, X_{k+1})\Big)$$

$$= \frac{1}{n}\sum_{k=0}^{n-1}\Big(\sum_{\tilde{x}\in A_{k+1}} \kappa(X_k, A_{k+1}, \tilde{x})\beta(X_k, A_{k+1}, \tilde{x}) - \beta(X_k, A_{k+1}, X_{k+1})\Big), \tag{21}$$

for β any real-valued measurable function defined on $E \times \mathcal{P} \times E$. We set $\mathcal{I}_n(f, \beta) = I_n(f) + \mathcal{J}_n(\beta)$. To prove the convergence and the asymptotic normality of the estimator $\mathcal{I}_n(f, \beta)$ of $\langle \pi, f\rangle$, we shall use a martingale approach. In particular, we shall assume there exists F a solution to the Poisson equation $F - PF = f - \langle \pi, f\rangle$ s.t. $\langle \pi, F^2\rangle < \infty$ (see theorem 17.4.2 and condition (V.3) p.341 in [8] to ensure the existence of such a solution).

We introduce the following convenient notation. For a probability measure ν on E and real valued functions h and g defined on E, we write, when well defined,

$$\mathrm{Cov}_\nu(h, g) = \langle \nu, gh\rangle - \langle \nu, g\rangle\langle \nu, h\rangle \quad \text{and} \quad \mathrm{Var}_\nu(h) = \langle \nu, h^2\rangle - \langle \nu, h\rangle^2$$

respectively the covariance of g and h and the variance of h w.r.t. ν. We also write $\kappa_{x,A}(dy)$ for the probability measure $\kappa(x, A, dy)$ and the $\beta_{x,A}(\cdot)$ for the function $\beta(x, A, \cdot)$.

Theorem 3.4. *We assume X is Harris recurrent, $\langle \pi, f^2\rangle < \infty$, there exists a solution F to the Poisson equation $F - PF = f - \langle \pi, f\rangle$ such that $\langle \pi, F^2\rangle < \infty$, and β is square integrable: $\int \pi(dx)\mathcal{Q}(x, dA)\kappa(x, A, dy)\beta(x, A, y)^2 < \infty$. Under those assumptions, we have:*

(i) *The estimator $\mathcal{I}_n(f, \beta)$ of $\langle \pi, f\rangle$ is consistent: a.s. $\lim_{n\to\infty} \mathcal{I}_n(f, \beta) = \langle \pi, f\rangle$.*

(ii) *The estimator $\mathcal{I}_n(f, \beta)$ of $\langle \pi, f\rangle$ is asymptotically normal:*

$$\sqrt{n}\left(I_n(f, \beta) - \langle \pi, f\rangle\right) \xrightarrow[n\to\infty]{(d)} \mathcal{N}(0, \sigma(f, \beta)^2),$$

and the asymptotic variance is given by

$$\sigma(f, \beta)^2 = \sigma(f)^2 + \int \pi(dx)\mathcal{Q}(x, dA)\left[\mathrm{Var}_{\kappa_{x,A}}(\beta_{x,A} - F) - \mathrm{Var}_{\kappa_{x,A}}(F)\right], \tag{22}$$

with $\sigma(f)^2 = \langle \pi, F^2 - (PF)^2\rangle$.

(iii) *The asymptotic variance $\sigma(f, \beta)^2$ is minimal for $\beta_{x,A} = F$ and*

$$\sigma(f, F)^2 = \int \pi(dx)\left(\int \mathcal{Q}(x, dA)\langle \kappa_{x,A}, F\rangle^2 - \left(\int \mathcal{Q}(x, dA)\langle \kappa_{x,A}, F\rangle\right)^2\right) \leq \sigma(f)^2. \tag{23}$$

Proof. We shall prove the Theorem when X_0 is distributed according to π. The general case follows from proposition 17.1.6 in [8], since X is Harris recurrent.

We set, for $n \geq 1$,

$$\Delta M_n = F(X_n) - PF(X_{n-1}) + \eta(X_{n-1}, A_n, X_n),$$

where

$$\eta(x, A, y) = \sum_{\tilde{x}\in A}\left(\kappa(x, A, \tilde{x}) - \mathbf{1}_{\{y=\tilde{x}\}}\right)\beta(x, A, \tilde{x}).$$

Notice that ΔM_n is square integrable and that $\mathbb{E}[\Delta M_{n+1}|\mathcal{G}_n] = 0$, where $\mathcal{G}_n$ is the σ-field generated by X_0 and (A_i, X_i) for $1 \leq i \leq n$. In particular $M = (M_n, n \geq 0)$ with $M_n =$

$\sum_{k=1}^n \Delta M_k$ is a martingale w.r.t. to the filtration $(\mathcal{G}_n, n \geq 0)$. Using that F solves the Poisson equation, we also have

$$\mathcal{I}_n(f,\beta) = \frac{1}{n} M_n - \frac{1}{n} PF(X_n) + \frac{1}{n} PF(X_0) + \langle \pi, f \rangle. \tag{24}$$

As $\langle \pi, F^2 \rangle < \infty$ implies that $\langle \pi, |PF| \rangle < \infty$, we deduce from theorem 17.3.3 in [8] that a.s. $\lim_{n\to\infty} \frac{1}{n} PF(X_n) = 0$. In particular part (i) of the Theorem will be proved as soon as we check that a.s. $\lim_{n\to\infty} \frac{1}{n} M_n = 0$.

We easily compute the bracket of M_n:

$$\langle M \rangle_n = \sum_{k=1}^n \mathbb{E}[\Delta M_k^2 | \mathcal{G}_{k-1}] = \sum_{k=1}^n h(X_{k-1}),$$

with

$$h(x) = P(F^2)(x) - (PF(x))^2 + \int \mathcal{Q}(x, dA) \left[-2\mathrm{Cov}_{\kappa(x,A,\cdot)}(\beta_{x,A}, F) + \mathrm{Var}_{\kappa(x,A,\cdot)}(\beta_{x,A}) \right].$$

Elementary computation yields

$$-2\mathrm{Cov}_{\kappa(x,A,\cdot)}(\beta_{x,A}, F) + \mathrm{Var}_{\kappa(x,A,\cdot)}(\beta_{x,A}) = \mathrm{Var}_{\kappa(x,A,\cdot)}(\beta_{x,A} - F) - \mathrm{Var}_{\kappa(x,A,\cdot)}(F).$$

Since $\langle \pi, F^2 \rangle < \infty$ and $\int \pi(dx)\mathcal{Q}(x,dA)\kappa(x,A,dy)\beta(x,A,y)^2 < \infty$, we have that h is π integrable. We set $\sigma(f,\beta)^2 = \langle \pi, h \rangle$, that is $\sigma(f,\beta)^2$ is given by (22), thanks to (5) and the fact that π is invariant for P. Theorem 17.3.2 in [8] asserts that a.s. $\lim_{n\to\infty} \frac{1}{n} \langle M \rangle_n = \langle \pi, h \rangle$. Then theorem 1.3.15 in [5] implies that a.s. $\lim_{n\to\infty} \frac{1}{n} M_n = 0$. This ends the proof of part (i).

The proof of part (ii) relies on the central limit theorem for martingales, see theorem 2.1.9 in [5]. We have already proved that a.s. $\lim_{n\to\infty} \frac{1}{n} \langle M \rangle_n = \sigma(f,\beta)^2$. Let us now check the Lindeberg's condition. Notice that theorem 17.3.2 in [8] implies that for any $a > 0$, we have

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^n \mathbb{E}[\Delta M_k^2 \mathbf{1}_{\{|\Delta M_k^2 > a\}} | \mathcal{G}_{k-1}] = \langle \pi, h_a \rangle,$$

where $h_a(x) = \mathbb{E}[\Delta M_1^2 \mathbf{1}_{\{|\Delta M_1^2 > a\}} | X_0 = x]$. Notice that $0 \leq h_a \leq h$ and that $(h_a, a > 0)$ decreases to 0 as a goes to infinity. We deduce that a.s.

$$\limsup_{n\to\infty} \frac{1}{n} \sum_{k=1}^n \mathbb{E}[\Delta M_k^2 \mathbf{1}_{\{|\Delta M_k^2 > \sqrt{n}\}} | \mathcal{G}_{k-1}] \leq \limsup_{a\to\infty} \langle \pi, h_a \rangle = 0.$$

This gives the Lindeberg's condition. We deduce then that $(\frac{1}{\sqrt{n}} M_n, n \geq 1)$ converges in distribution to $\mathcal{N}(0, \sigma(f,\beta)^2)$. Then use (24) and that a.s. $\lim_{n\to\infty} \frac{1}{n}(PF(X_{n+1}))^2 = 0$ (thanks to theorem 17.3.3 in [8]) to get part (ii).

Proof of part (iii). The asymptotic variance $\sigma(f,\beta)^2$ is minimal when $\mathrm{Var}_{\kappa_{x,A}}(\beta_{x,A} - F) = 0$ that is at least for $\beta_{x,A} = F$. Of course, $\sigma(f,F)^2 \leq \sigma(f,0)^2 = \sigma(f)^2$. Using (5), that π is invariant for P and the definition (20) of P, we get

$$\begin{aligned} \sigma(f)^2 &= \langle \pi, PF^2 \rangle - \langle \pi, (PF)^2 \rangle \\ &= \int \pi(dx)\mathcal{Q}(x,dA)\langle \kappa_{x,A}, F^2 \rangle - \int \pi(dx) \left(\int \mathcal{Q}(x,dA)\langle \kappa_{x,A}, F \rangle \right)^2. \end{aligned}$$

And the expression of $\sigma(f,F)^2$ follows from (22).

$\square$

4. The Boltzmann case

We work in the general setting of Section 3 with the Boltzmann selection kernel κ given by (19) (or simply (15) when E is finite). The next Proposition generalizes Proposition 2.8. It ensures that the asymptotic variance of the waste recycling algorithm $\sigma(f,f)^2$ is smaller than the one $\sigma(f)^2$ of the standard Metropolis Hastings algorithm and that $b \mapsto \sigma(f,bf)^2$ is minimal at $b_\star$ given by (7). In the same time, we show that this variance $\sigma(f)^2$ is at least divided by two for the optimal choice $\beta(x,A,y) = F(y)$ in our control variate approach.

For f s.t. $\langle \pi, f^2 \rangle < \infty$, we set $f_0 = f - \langle \pi, f \rangle$ and

$$\Delta(f) = \frac{1}{2} \int \pi(dx) P(x,dy) (f_0(x) + f_0(y))^2 = \langle \pi, f_0(f_0 + Pf_0) \rangle. \tag{25}$$

Notice that the second equality in (25) is a consequence of the invariance of π w.r.t. P.

Proposition 4.1. *We assume that X is Harris recurrent, $\langle \pi, f^2 \rangle < \infty$, there exists a solution F to the Poisson equation $F - PF = f - \langle \pi, f \rangle$ such that $\langle \pi, F^2 \rangle < \infty$. We consider the Boltzmann case: the selection kernel κ is given by (19). For $\beta(x,A,y)$ respectively equal to $F(y)$ and $f(y)$, one has*

$$\sigma(f,F)^2 = \frac{1}{2}\Big(\sigma(f)^2 - \mathrm{Var}_\pi(f)\Big) \text{ and } \sigma(f,f)^2 = \sigma(f)^2 - \Delta(f).$$

The non-negative term $\Delta(f)$ is positive when $\mathrm{Var}_\pi(f) > 0$.

Furthermore, if $\mathrm{Var}_\pi(f) > 0$, then $\langle \pi, f^2 - fPf \rangle = \frac{1}{2}\mathbb{E}_\pi\left[(f(X_0) - f(X_1))^2\right]$ is positive, the function $b \mapsto \sigma(f,bf)^2$ is minimal at

$$b_\star = \frac{\langle \pi, f^2 \rangle - \langle \pi, f \rangle^2}{\langle \pi, f^2 - fPf \rangle}, \tag{26}$$

and $b_\star > 1$ when $\sigma(f,f)^2 > 0$.

Proof. Recall notations from Example 3.1. We set $\kappa_A^B(dy) = \kappa^B(A,dy)$. For g and h real valued functions defined on E, we have

$$\begin{aligned} \int \pi(dx) \mathcal{Q}(x,dA)\, \langle \kappa_A^B, g \rangle \langle \kappa_A^B, h \rangle &= \int N_0(dA) r_A(dx)\, \langle \kappa_A^B, g \rangle \langle \kappa_A^B, h \rangle \\ &= \int N_0(dA)\, \langle r_A, g \rangle \langle \kappa_A^B, h \rangle \\ &= \int \pi(dx) \mathcal{Q}(x,dA)\, g(x) \langle \kappa_A^B, h \rangle \\ &= \langle \pi, gPh \rangle, \end{aligned} \tag{27}$$

where we used (19) for the second equality. Using this equality with $h = g = F$ in the first term of the expression of $\sigma(f,F)^2$ given in (23), we obtain

$$\sigma(f,F)^2 = \langle \pi, FPF - (PF)^2 \rangle = \frac{1}{2}\langle \pi, F^2 - (PF)^2 - (F - PF)^2 \rangle = \frac{1}{2}(\sigma(f)^2 - \mathrm{Var}_\pi(f)),$$

where we used the Poisson equation (6) for the last equality.

We also get that

$$\begin{aligned}
\int \pi(dx)\mathcal{Q}(x,dA)\left[\mathrm{Var}_{\kappa_A^B}(bf-F)-\mathrm{Var}_{\kappa_A^B}(F)\right]&\\
= \int \pi(dx)\mathcal{Q}(x,dA)\big[\langle\kappa_A^B,(bf-F)^2\rangle &- \langle\kappa_A^B, bf\rangle^2 + 2\langle\kappa_A^B,bf\rangle\langle\kappa_A^B,F\rangle\\
&-\langle\kappa_A^B,F\rangle^2 - \langle\kappa_A^B,F^2\rangle + \langle\kappa_A^B,F\rangle^2\big]\\
= \langle\pi, b^2f^2 - 2bfF - b^2fPf + 2fPF\rangle&\\
= b^2\langle\pi, f^2 - fPf\rangle - 2b\left(\langle\pi,f^2\rangle - \langle\pi,f\rangle^2\right),&
\end{aligned}$$

where we used (27) for the second equation and (6) for the last equality. We deduce from (22) with $\beta_{x,A} = bf$ that

$$\sigma(f,bf)^2 - \sigma(f)^2 = b^2\langle\pi, f^2 - fPf\rangle - 2b\left(\langle\pi,f^2\rangle - \langle\pi,f\rangle^2\right).$$

We first check that $\mathrm{Var}_\pi(f) > 0$ implies that $\langle\pi, f^2 - fPf\rangle > 0$. If, when X_0 is distributed according to π, a.s. $f(X_1) = f(X_0)$, then a.s. $k \mapsto f(X_k)$ is constant and by the ergodic theorem this constant is equal to $\langle\pi, f\rangle$. Therefore $\mathrm{Var}_\pi(f) > 0$ implies positivity of $\langle\pi, f^2 - fPf\rangle$ which is equal to $\frac{1}{2}\mathbb{E}_\pi\left[(f(X_0) - f(X_1))^2\right]$ by reversibility of π w.r.t. P.

Hence when $\mathrm{Var}_\pi(f) > 0$, then $b \mapsto \sigma(f,bf)^2$ is minimal for $b = b_\star$ defined by (26).

For the choice $b = 1$, one obtains

$$-\sigma(f,f)^2 + \sigma(f)^2 = \langle\pi, f(f+Pf)\rangle - 2\langle\pi,f\rangle^2 = \Delta(f) = \mathrm{Var}_\pi(f) + \langle\pi, f_0Pf_0\rangle. \tag{28}$$

By (27), $\langle\pi, f_0Pf_0\rangle = \int \pi(dx)\mathcal{Q}(x,dA)\langle\kappa_A^B, f_0\rangle^2 \geq 0$ and $\Delta(f)$ is positive when $\mathrm{Var}_\pi(f) > 0$.

Moreover the difference $\langle\pi, fPf\rangle - \langle\pi,f\rangle^2 = \langle\pi, f_0Pf_0\rangle$ is non-negative thanks to (27) and when it is equal to 0, then (27) implies that $\langle\pi, f_0Pg\rangle = \langle\pi, gPf_0\rangle = 0$ for each function g on E such that $\langle\pi, g^2\rangle < +\infty$. In this case, by (28),

$$\begin{aligned}
\sigma(f,f)^2 &= \sigma(f)^2 + \sigma(f,f)^2 - \sigma(f)^2\\
&= \langle\pi, (F+PF)(F-PF)\rangle - \mathrm{Var}_\pi(f)\\
&= \langle\pi, (f_0 + 2PF)f_0\rangle - \mathrm{Var}_\pi(f) = 0.
\end{aligned}$$

Hence when $\mathrm{Var}_\pi(f) > 0$ and $\sigma(f,f)^2 > 0$ then, we have $\langle\pi, f_0Pf_0\rangle > 0$ and $b_\star > 1$. □

5. Further results in the single-proposal case

The Metropolis-Hastings algorithm corresponds to the single proposal case that is the particular case of the multi-proposal algorithm of Section 3 where $\mathcal{Q}(x,.)$ gives full weight to the set of subsets of E (not assumed to be finite) containing x and at most one other element of E. The acceptance probability is then given by $\rho(x,y) = \kappa(x,\{x,y\},y)$ and the selection kernel $Q(x,.)$ is the image of $\mathcal{Q}(x,.)$ by any measurable mapping such that the image of $\{x,y\}$ is y. See Remark (2.6) in the particular case of E finite. Equation (17) is then equivalent to the following generalization of (1)

$$\pi(dx)Q(x,dy)\rho(x,y) = \pi(dy)Q(y,dx)\rho(y,x). \tag{29}$$

Moreover the transition kernel of the Markov chain X is given by

$$\mathbf{1}_{\{y\neq x\}}P(x,dy) = \mathbf{1}_{\{y\neq x\}}\rho(x,y)Q(x,dy) \text{ and } P(x,\{x\}) = 1 - \int_{z\neq x}\rho(x,z)Q(x,dz). \tag{30}$$

Motivated by the study of the WR algorithm which corresponds to $\psi = f$ and of the optimal choice $\psi = F$, we are first going to derive more convenient expressions of $\sigma(f,\psi)^2$ in the single proposal framework. We then use this new expression to construct a counter-example such that $\sigma(f,f)^2 > \sigma(f)^2$. And, when $\rho(x,y)+\rho(y,x)$ is constant on $E_*^2 = E^2 \setminus \{(x,x) : x \in E\}$, using again the expression of $\sigma(f,\psi)^2$, we compute the value of b such that $\sigma(f,bf)^2$ is minimal and check that $\sigma(f,f)^2 < \sigma(f)^2$ as soon as f is non constant.

5.1. **Another expression of the asympotic variance.** We recall that in the notation $\mathbb{E}_\pi$, the subscript π means that X_0 is distributed according to π.

Lemma 5.1. *We assume that $\langle \pi, f^2\rangle < \infty$ and there exists a solution F to the Poisson equation* (6) *such that $\langle \pi, F^2\rangle < +\infty$. Let ψ be square integrable: $\langle \pi, \psi^2\rangle < \infty$. In the single proposal case, we have*

$$\sigma(f,\psi) = \sigma(f)^2 - \mathbb{E}_\pi\left[\Big(1-\rho(X_0,X_1)\Big)\Big(F(X_1)-F(X_0)\Big)^2\right] + \mathbb{E}_\pi\left[\Big(1-\rho(X_0,X_1)\Big)\Big(\psi(X_1)-F(X_1)-\psi(X_0)+F(X_0)\Big)^2\right].$$

Proof. In the single proposal case, $\kappa(x,\{x,y\},y) = 1-\kappa(x,\{x,y\},x) = \rho(x,y)$ for $x \neq y$. Therefore, for a real valued function g defined on E, we have

$$\mathrm{Var}_{\kappa(x,\{x,y\},.)}(g) = \rho(x,y)(1-\rho(x,y))(g(y)-g(x))^2. \tag{31}$$

Thus we deduce that

$$\begin{aligned}\int_{E_*^2} \pi(dx)Q(x,dy)\mathrm{Var}_{\kappa(x,\{x,y\},.)}(g) &= \int_{E_*^2} \pi(dx)Q(x,dy)\rho(x,y)(1-\rho(x,y))(g(y)-g(x))^2\\ &= \int_{E_*^2} \pi(dx)P(x,dy)(1-\rho(x,y))(g(y)-g(x))^2\\ &= \mathbb{E}_\pi\left[\Big(1-\rho(X_0,X_1)\Big)\Big(g(X_1)-g(X_0)\Big)^2\right].\end{aligned}$$

where we used (30) for the second equality. Plugging this formula with $g = \psi - F$ and $g = F$ in (22) gives the result. $\square$

Taking $\psi = F$ and $\psi = f$ in the previous Lemma gives the following Corollary.

Corollary 5.2. *We assume that $\langle \pi, f^2\rangle < \infty$ and there exists a solution F to the Poisson equation* (6) *such that $\langle \pi, F^2\rangle < +\infty$. In the single proposal case, we have:*

$$\sigma(f,F)^2 - \sigma(f)^2 = -\mathbb{E}_\pi\left[(1-\rho(X_0,X_1))(F(X_1)-F(X_0))^2\right],$$
$$\sigma(f,f)^2 - \sigma(f)^2 = -\mathbb{E}_\pi\left[(1-\rho(X_0,X_1))\left[(F(X_1)-F(X_0))^2 - (PF(X_1)-PF(X_0))^2\right]\right].$$

5.2. **A counter-example.** We are going to construct a counter-example such that $\sigma(f,f)^2 > \sigma(f)^2$ in the Metropolis case, thus proving the statements concerning this case in Proposition 2.3. This counter-example is also such that the optimal choice $\psi = F$ does not achieve variance reduction : $\sigma(f,F)^2 = \sigma(f)^2$. Let P be an irreducible transition matrix on $E = \{a,b,c\}$, with invariant probability measure π s.t. P is reversible w.r.t. π,

$$P(a,b) > 0,\ P(a,a) > 0 \text{ and } P(a,c) \neq P(b,c).$$

Let f be defined by $f(x) = \mathbf{1}_{\{x=c\}} - P(x,c)$ for $x \in E$. We have

$$\langle \pi, f\rangle = \pi(c) - \sum_{x\in E} \pi(x)P(x,c) = 0.$$

The function $F(x) = \mathbf{1}_{\{x=c\}}$ solves the Poisson equation (6): $F - PF = f - \langle \pi, f\rangle$.

Let $\rho \in \left(\frac{P(a,b)}{P(a,a)+P(a,b)}, 1\right)$. We set

$$Q(x,y) = \begin{cases} \frac{P(a,b)}{\rho} \text{ if } (x,y) = (a,b), \\ P(a,a) - P(a,b)(\frac{1}{\rho} - 1) \text{ if } (x,y) = (a,a), \\ P(x,y) \text{ otherwise.} \end{cases}$$

We choose

$$\rho(x,y) = \begin{cases} \rho \text{ if } (x,y) = (a,b), \\ 1 \text{ otherwise.} \end{cases}$$

Since $\rho(a,b)\pi(a)Q(a,b) = \rho\pi(a)P(a,b)/\rho$, we have $\rho(x,y)\pi(x)Q(x,y) = \pi(x)P(x,y)$ for all $x \neq y \in E$. Equation (1) follows from the reversibility of π for P. Notice also that (2) holds with $\gamma(u) = \min(1,u)$.

By construction, the matrix P satisfies (3). By Corollary 5.2, we have $\sigma(f,F)^2 - \sigma(f)^2 = 0$ and

$$\sigma(f,f)^2 - \sigma(f)^2 = \pi(a)P(a,b)(1-\rho)(P(b,c) - P(a,c))^2 > 0. \tag{32}$$

Let us illustrate these results by simulation for the following specific choice

$$\pi = \frac{1}{10}\begin{pmatrix} 6 \\ 3 \\ 1 \end{pmatrix}, \; P = \frac{1}{60}\begin{pmatrix} 38 & 21 & 1 \\ 42 & 0 & 18 \\ 6 & 54 & 0 \end{pmatrix}, \; \rho = \frac{4}{10} \text{ and } Q = \frac{1}{120}\begin{pmatrix} 13 & 105 & 2 \\ 84 & 0 & 36 \\ 12 & 108 & 0 \end{pmatrix}.$$

Then $\sigma(f)^2 - \sigma(f,f)^2 = -0.010115$ amounts to 14% of $\sigma(f)^2 \simeq 0.0728333$.

Using $N = 10\,000$ simulations, we give estimations of the variances σ_n^2 of $I_n(f)$, $\sigma_{WR,n}^2$ of $I_n(f,f)$ and of the difference $\sigma_n^2 - \sigma_{WR,n}^2$ with asymptotic confidence intervals at level 95%. The initial variable X_0 is generated according to the reversible probability measure π.

n	σ_n^2	$\sigma_{WR,n}^2$	$\sigma_n^2 - \sigma_{WR,n}^2$
1	[0.1213 , 0.1339]	[0.1116 , 0.1241]	[0.0091 , 0.0104]
2	[0.0728 , 0.0779]	[0.0758 , 0.0815]	[-0.0041 , -0.0025]
5	[0.0733 , 0.0791]	[0.0798 , 0.0859]	[-0.0075 , -0.0058]
10	[0.0718 , 0.0772]	[0.0800 , 0.0859]	[-0.0094 , -0.0074]
100	[0.0702 , 0.0751]	[0.0803 , 0.0858]	[-0.0114 , -0.0092]
1000	[0.0719 , 0.0769]	[0.0811 , 0.0867]	[-0.0105 , -0.0083]

5.3. **Case of a constant sum $\rho(x,y) + \rho(y,x)$.** Under Boltzmann selection rule, according to Proposition 4.1, the asymptotic variance $\sigma(f,f)^2$ of $I_n^{WR}(f) = I_n(f,f)$ is smaller than the one $\sigma(f)^2$ of $I_n(f)$ and $\sigma(f,bf)$ is minimal for $b = b_\star$ given by (26). In the single proposal case, Boltzmann selection rule ensures that $\rho(x,y)+\rho(y,x) = 1$ on $E_*^2 = E^2 \setminus \{(x,x) : x \in E\}$. It turns out that we are still able to prove the same results as soon as $\rho(x,y) + \rho(y,x)$ is constant on E_*^2. Notice that $\mathrm{Var}_\pi(f) \geq 0$ and that the trivial case $\mathrm{Var}_\pi(f) = 0$ corresponds to f constant π-a.s..

Proposition 5.3. *We assume $\langle \pi, f^2 \rangle < \infty$, $\mathrm{Var}_\pi(f) > 0$, there exists a solution F to the Poisson equation (6) such that $\langle \pi, F^2 \rangle < \infty$. We consider the single proposal case and assume that there exists $\alpha \in (0,2)$ such that*

$$\pi(dx)Q(x,dy) \text{ a.e. on } E_*^2, \; \rho(x,y) + \rho(y,x) = \alpha. \tag{33}$$

Then we have:

i) $\langle \pi, f^2 - fPf \rangle = \frac{1}{2}\mathbb{E}_\pi\left[(f(X_0) - f(X_1))^2\right]$ *is positive.*

ii)

$$\sigma(f,\psi)-\sigma(f)^2 = -(1-\alpha/2)\mathbb{E}_\pi\left[\Big(F(X_1)-F(X_0)\Big)^2\right] + (1-\alpha/2)\mathbb{E}_\pi\left[\Big(\psi(X_1)-F(X_1)-\psi(X_0)+F(X_0)\Big)^2\right], \tag{34}$$

for any real valued function ψ on E such that $\langle\pi,\psi^2\rangle<\infty$.

iii) *The function $b\mapsto\sigma(f,bf)^2$ is minimal at $b_\star$ given by (26) and $b_\star\geq 1/\alpha$.*

iv) $\sigma(f,f)^2-\sigma(f)^2=-(2-\alpha)\Delta(f)<0$, *where $\Delta(f)$ is given by (25).*

Proof. Statement i) follows from the proof of Proposition 4.1.

For statement ii), notice that by reversibility of π, we deduce from Lemma 5.1 that

$$\sigma(f,\psi)-\sigma(f)^2 = -\mathbb{E}_\pi\left[\Big(1-\rho(X_1,X_0)\Big)\Big(F(X_1)-F(X_0)\Big)^2\right] + \mathbb{E}_\pi\left[\Big(1-\rho(X_1,X_0)\Big)\Big(\psi(X_1)-F(X_1)-\psi(X_0)+F(X_0)\Big)^2\right].$$

This and Lemma 5.1 imply (34).

For iii), using (34) with $\psi=bf$, it is straightforward to get that $\sigma(f,bf)^2$ is minimal when b equals

$$\frac{\mathbb{E}_\pi\left[(f(X_1)-f(X_0))(F(X_1)-F(X_0))\right]}{\mathbb{E}_\pi\left[(f(X_1)-f(X_0))^2\right]} = \frac{\langle\pi,f(F-PF)\rangle}{\langle\pi,f^2-fPf\rangle} = \frac{\langle\pi,f^2\rangle-\langle\pi,f\rangle^2}{\langle\pi,f^2-fPf\rangle} = b_\star.$$

Remarking that $b_\star=\frac{\langle\pi,f_0^2\rangle}{\langle\pi,f_0^2-f_0Pf_0\rangle}=\frac{\langle\pi,f_0^2\rangle}{\alpha\langle\pi,f_0^2\rangle-\langle\pi,f_0Pf_0+(\alpha-1)f_0^2\rangle}$ and using Lemma 5.4 below, one deduce that $b_\star\geq 1/\alpha$.

We now prove iv). Recall that $f_0=f-\langle\pi,f\rangle$. Since $\langle\pi,f_0(f_0+Pf_0)\rangle=(2-\alpha)\mathrm{Var}_\pi(f)+\langle\pi,f_0Pf_0+(\alpha-1)f_0^2\rangle$, we deduce from Lemma 5.4 that $\Delta(f)$ given by (25) is positive. We have

$$\begin{aligned}
\frac{1}{2}\,\mathbb{E}_\pi&\left[(f(X_1)-F(X_1)-f(X_0)+F(X_0))^2-(F(X_1)-F(X_0))^2\right]\\
&=\frac{1}{2}\,\mathbb{E}_\pi\left[(f_0(X_1)-f_0(X_0))^2\right]-\mathbb{E}_\pi\left[(f_0(X_1)-f_0(X_0))(F(X_1)-F(X_0))\right]\\
&=\langle\pi,f_0^2-f_0Pf_0\rangle-2\langle\pi,f_0(F-PF)\rangle\\
&=-\langle\pi,f_0(f_0+Pf_0)\rangle,
\end{aligned}$$

where we used that π is invariant for P and that P is reversible with respect to π for the second equality and that F solves (6) for the last equality. We conclude using (34) with $\psi=f$. □

Lemma 5.4. *Let h be a real valued function defined on E such that $\langle\pi,h^2\rangle<\infty$. Under hypothesis (33), we have $\langle\pi,hPh+(\alpha-1)h^2\rangle\geq 0$.*

Proof. Using (30) then (33), we obtain

$$\begin{aligned}\langle \pi, hPh + (\alpha-1)h^2\rangle &= \int_{E_*^2} \pi(dx)Q(x,dy)\rho(x,y)h(x)h(y) \\ &\qquad + \int_E \pi(dx)\left(\alpha - \int_E \mathbf{1}_{y\neq x} Q(x,dy)\rho(x,y)\right) h^2(x) \\ &= \int_{E_*^2} \pi(dx)Q(x,dy)\left[\rho(x,y)h(x)h(y) + \rho(y,x)h^2(x)\right] \\ &\qquad + \alpha \int_E \pi(dx)Q(x,\{x\})h^2(x).\end{aligned}$$

To conclude, it is enough to check that the first term in the r.h.s. is nonnegative. Using (33) and (29) for the first equality, we get

$$\begin{aligned}&\alpha \int_{E_*^2} \pi(dx)Q(x,dy)\left[\rho(x,y)h(x)h(y) + \rho(y,x)h^2(x)\right] \\ &\qquad = \int_{E_*^2} \pi(dx)Q(x,dy)\rho(y,x)\left[\rho(x,y)h(x)h(y) + \rho(y,x)h^2(x)\right] \\ &\qquad\qquad + \int_{E_*^2} \pi(dy)Q(y,dx)\rho(y,x)\left[\rho(x,y)h(x)h(y) + \rho(y,x)h^2(x)\right] \\ &\qquad = \int_{E_*^2} \pi(dx)Q(x,dy)\left[\rho(y,x)h(x) + \rho(x,y)h(y)\right]^2 \\ &\qquad \geq 0.\end{aligned}$$

□

6. Other remarks

We work in the general setting of Section 3.

6.1. **About the estimator $I_n(f + P\psi - \psi)$.** Motivated by Remark 2.5 on the study of $I_n(f + P\psi - \psi)$, we compute the asymptotic variance $\tilde\sigma(f,\beta)^2$ of

$$\begin{aligned}&I_n(f) + \frac{1}{n}\sum_{k=0}^{n-1} \left(\int \mathcal{Q}(X_k, dA)\kappa(X_k, A, d\tilde x)\beta(X_k, A, \tilde x) - \beta(X_k, A_{k+1}, X_{k+1})\right) \\ &\qquad = I_n(f) + \frac{1}{n}\sum_{k=0}^{n-1}\Big(\mathbb{E}[\beta(X_k, A_{k+1}, X_{k+1})|X_k] - \beta(X_k, A_{k+1}, X_{k+1})\Big).\end{aligned}$$

Following the proof of Theorem 3.4, one obtains that the above estimator of $\langle \pi, f\rangle$ is under the hypotheses of Theorem 3.4 convergent and asymptotically normal with asymptotic variance

$$\tilde\sigma(f,\beta)^2 = \sigma(f,\beta)^2 + \int \pi(dx)\left[\mathrm{Var}_{\mathcal{Q}(x,.)}(\kappa\beta_x - \kappa F_x) - \mathrm{Var}_{\mathcal{Q}(x,.)}(\kappa F_x)\right],$$

where $\mathrm{Var}_{\mathcal{Q}(x,\cdot)}(\varphi) = \int \mathcal{Q}(x,dA)\varphi(A)^2 - \left(\int \mathcal{Q}(x,dA)\varphi(A)\right)^2$, $\kappa\beta_x(A) = \langle \kappa_{x,A}, \beta_{x,A}\rangle$ and $\kappa F_x(A) = \langle \kappa_{x,A}, F\rangle$.

Notice that the sign of $\tilde\sigma(f,\beta)^2 - \sigma(f,\beta)^2$ depends on β (take $\beta_{x,A} = F$ and $\beta_{x,A} = -F$).

6.2. **Changing the selection kernel in $\mathcal{J}_n$.** Let $\kappa' \neq \kappa$ be such that (17) (or simply (10) if E is finite) still holds when κ is replaced by κ' and $\mathcal{J}'_n(\psi)$ and $\mathcal{J}'_n(\beta)$ be defined like $\mathcal{J}_n(\psi)$ and $\mathcal{J}_n(\beta)$ with the chain X unchanged but with $\kappa(X_k, A_{k+1}, \tilde{x})$ replaced by $\kappa'(X_k, A_{k+1}, \tilde{x})$ in (12) and (21). Thus, we have

$$\mathcal{J}'_n(\psi) = \frac{1}{n}\sum_{k=0}^{n-1} \sum_{\tilde{x}\in A_{k+1}} \left(\kappa'(X_k, A_{k+1}, \tilde{x}) - \mathbf{1}_{\{X_{k+1}=\tilde{x}\}}\right) \psi(\tilde{x}).$$

Note that in general $\sum_{\tilde{x}\in A_{k+1}} \kappa'(X_k, A_{k+1}, \tilde{x})\psi(\tilde{x}) \neq \mathbb{E}[\psi(X_{k+1})|X_k, A_{k+1}]$.

In the single proposal case, Frenkel [7] suggests that $\mathcal{J}'_n(f)$ can also be used as a control variate. In general, for a real valued function β defined on $E \times \mathcal{P} \times E$, the almost sure limit of $\mathcal{J}'_n(\beta)$ is different from zero, which means the estimator $I_n(f) + \mathcal{J}'_n(\beta)$ of $\langle \pi, f\rangle$ is not convergent. However, when $\beta(x, A, \cdot) = \psi(\cdot)$, Lemma 6.1 below ensures that the estimator $I_n(f) + \mathcal{J}'_n(\psi)$ of $\langle \pi, f\rangle$ is convergent. It is also easy to prove that this estimator is asymptotically normal and compute the asymptotic variance, but we have not been able to compare it with the asymptotic variance $\sigma(f)^2$ of $I_n(f)$.

Lemma 6.1. *We assume X is Harris recurrent, $\langle \pi, f^2\rangle < \infty$, there exists a solution F to the Poisson equation $F - PF = f - \langle \pi, f\rangle$ such that $\langle \pi, F^2\rangle < \infty$, and ψ is such that: $\langle \pi, \psi^2\rangle < \infty$. Under those assumptions, the estimator $I_n(f) + \mathcal{J}'_n(\psi)$ of $\langle \pi, f\rangle$ is consistent: a.s. $\lim_{n\to\infty} I_n(f) + \mathcal{J}'_n(\psi) = \langle \pi, f\rangle$.*

Proof. We set

$$\Delta R_n = \int \kappa'(X_{n-1}, A_n, d\tilde{x})\psi(\tilde{x}) - \int \mathcal{Q}(X_{n-1}, dA)\kappa'(X_{n-1}, A, d\tilde{x})\psi(\tilde{x}).$$

Notice that ΔR_n is square integrable and that $\mathbb{E}[\Delta R_{n+1}|\mathcal{G}_n] = 0$, where $\mathcal{G}_n$ is the σ-field generated by X_0 and (A_i, X_i) for $1 \leq i \leq n$. In particular $R = (R_n, n \geq 0)$ with $R_n = \sum_{k=1}^n \Delta R_k$ is a martingale w.r.t. to the filtration $(\mathcal{G}_n, n \geq 0)$. Notice that

$$\mathcal{J}'_n(\psi) = \frac{1}{n} R_n + I_n(\gamma) - \frac{1}{n}\int \mathcal{Q}(X_n, dA)\kappa'(X_n, A, d\tilde{x})\psi(\tilde{x}) + \frac{1}{n}\int \mathcal{Q}(X_0, dA)\kappa'(X_0, A, d\tilde{x})\psi(\tilde{x}),$$

where $\gamma(x) = \int \mathcal{Q}(x, dA)\kappa'(x, A, d\tilde{x})\psi(\tilde{x}) - \psi(x)$. Following the proof of Theorem 3.4, we easily get that a.s. $\lim_{n\to\infty} \frac{1}{n} R_n = 0$ and that a.s.

$$\lim_{n\to\infty} \mathcal{J}'_n(\psi) = \lim_{n\to\infty} I_n(\gamma) = \langle \pi, \gamma\rangle.$$

Using (17) satisfied by κ' instead of κ, we get that $\langle \pi, \gamma\rangle = 0$. This ends the proof of the Lemma. □

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